L5 ANSWER 1 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2005:244468 CAPLUS Full-text

DN 143:3506

TI Fluorescent metal ion indicators based on benzoannelated crown systems: a green fluorescent indicator for intracellular sodium ions

AU Martin, Vladimir V.; Rothe, Anca; Gee, Kyle R.

CS Molecular Probes Invitrogen Detection Technologies, Eugene, OR, 97402, USA

SO Bioorganic & Medicinal Chemistry Letters (2005), 15(7), 1851-1855 CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier B.V.

DT Journal

LA English

The synthesis and metal binding properties of cation-sensitive fluorescent indicators intended for biol. applications are described. The increase of the crown ether ring size enhances the affinity for larger cations, but weakens the fluorescent response and selectivity. A compound having a 15-crown-5 chelator directly attached to a 2,7-difluoroxanthenone fluorophore loads into live cells and responds to sodium ion concentration changes with large fluorescence increases in the visible wavelength range.

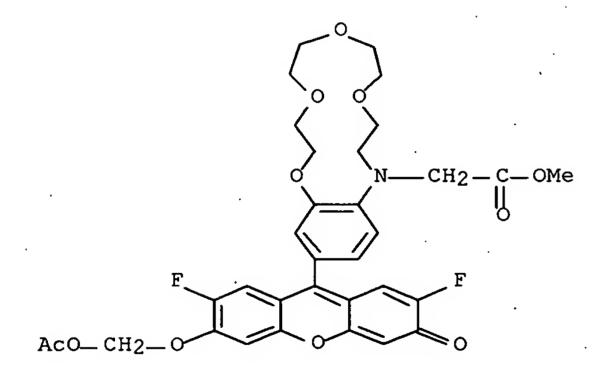
IT **690993-67-0P**, CoroNA Green AM

RL: ARG (Analytical reagent use); BUU (Biological use, unclassified); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); USES (Uses)

(fluorescent metal ion indicators based on benzoannelated crown systems and a green fluorescent indicator for intracellular sodium ions)

RN 690993-67-0 CAPLUS

CN 13H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-13-acetic acid, 16-[6-[(acetyloxy)methoxy]-2,7-difluoro-3-oxo-3H-xanthen-9-yl]-2,3,5,6,8,9,11,12-octahydro-, methyl ester (9CI) (CA INDEX NAME)



RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 2 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN
L5
```

2005:158631 CAPLUS Full-text AN

142:261567 DN

Preparation of crown ether derivatives as metal chelating agents ΤI

Gee, Kyle; Martin, Vladimir IN

Molecular Probes, Inc., USA PA

PCT Int. Appl., 136 pp. SO

CODEN: PIXXD2

DT Patent

English FAN.CNT 1

LA

	PATENT NO.				KIND DATE			APPLICATION NO.					DATE					
ΡI	WO 2005016874			A2 20050224		WO 2003-US24662						20030804						
		W:	AE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
•.			CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
			GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,
			LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	NZ,	OM,
			PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	TJ,	TM,	TN,
			ŤR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW			
		RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	AZ,	BY,
			KG,	KZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,
			FI,	FR,	GB,	GR,	HU,	IE,	IT,	LU,	MC,	NL,	PT,	RO,	SE,	SI,	SK,	TR,
			BF,	BJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG
PRAI GI	WO	2003	-US2	4662				2003	0804									

$$R^7$$
 $N-E^2-Y-E^3-O$
 R^{19}
 R^{19}
 R^{10}
 R^{10}
 R^{19}
 R^{19}
 R^{10}
 R^{10}

The invention describes crown ether chelators having the formula (I) [Y, P, Q AB = 0, S, (un) substituted NH, absent;, L is independently a covalent linkage; each Rx is independently a reactive group; E1, E2, E3 = independently -[C(R5)2]n-, -(COCH2)n-, -[C(R5)2]nO[C(R5).2]n; or E2 is absent; where n = 2, 3 or 4; R5 = independently H or Me, or two R5 moieties on adjacent carbons of one or more of E1, E2 or E3, when taken in combination, form a 5- or 6membered aliphatic ring; R1 = each (un)substituted -L-Rx, -L-Sc, -L-DYE, C1-18 alkyl, or C7-18 arylalkyl; R7, R8, R9, R10, R19, R20 = H, halogen, azido, nitro, nitroso, amino, cyano, each (un) substituted -L-Rx, -L-Sc, -L-DYE, C1-6 alkyl, or C1-6 alkoxy; or R19 and R20 taken in combination form an (un) substituted fused six-membered benzo moiety; or any two adjacent substituents R7-R10, taken in combination, form an (un) substituted fused sixmembered benzo moiety; or any two adjacent substituents R7-R10, or R19 and R20, taken in combination with each other, form a fused DYE; wherein L = acovalent linkage; Sc = a conjugated substance; DYE = a reporter mol.] and azasubstituted and thia-substituted analogs thereof. These crown ethers may be

substituted by a dye moiety, a chemical reactive group, a conjugated substance, or a combination thereof. Chelators that are substituted by fluorescent dyes, e.g. (II), are particularly useful as indicators for metal cations, particularly Na+ and K+ ions, and particularly where binding of the target ion results in a change in the fluorescence properties of the indicator that can be correlated with the ion concentration Methods are provided for utilizing reactive groups on the chelators for conjugation to dyes, lipids and polymers and methods for enhancing entry of the indicators into living cells.

IT 690993-67-0P 690993-68-1P 690993-69-2P 690993-90-9P 690993-91-0P 690993-93-2P 690994-00-4P 690994-01-5P 846023-88-9P

RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)

(preparation of crown ether derivs. as metal chelating agents or fluorescence indicators)

RN 690993-67-0 CAPLUS

CN 13H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-13-acetic acid, 16-[6-[(acetyloxy)methoxy]-2,7-difluoro-3-oxo-3H-xanthen-9-yl]-2,3,5,6,8,9,11,12-octahydro-, methyl ester (9CI) (CA INDEX NAME)

RN 690993-68-1 CAPLUS

CN Xanthylium, 3,6-bis(dimethylamino)-9-[2,3,5,6,8,9,12,13-octahydro-13-(2-methoxy-2-oxoethyl)-11H-1,4,7,10,13-benzotetraoxaazacyclopentadecin-16-yl]-(9CI) (CA INDEX NAME)

RN 690993-69-2 CAPLUS

CN Boron, difluoro[methyl 16-[(3,5-dimethyl-1H-pyrrol-2-yl-κN)(3,5-dimethyl-2H-pyrrol-2-ylidene-κN)methyl]-2,3,5,6,8,9,11,12-octahydro-13H-1,4,7,10,13-benzotetraoxaazacyclopentadecine-13-acetato]-, (T-4)-(9CI) (CA INDEX NAME)

RN 690993-90-9 CAPLUS

CN 3H-Xanthen-3-one, 6-[(acetyloxy)methoxy]-2,7-difluoro-9-[2,3,5,6,8,9,12,13-octahydro-13-(2-methoxyethyl)-11H-1,4,7,10,13-benzotetraoxaazacyclopentadecin-16-yl]- (9CI) (CA INDEX NAME)

RN 690993-91-0 CAPLUS

CN Xanthylium, 3,6-bis(dimethylamino)-9-[2,3,5,6,8,9,12,13-octahydro-13-(2-methoxyethyl)-11H-1,4,7,10,13-benzotetraoxaazacyclopentadecin-16-yl]-(9CI) (CA INDEX NAME)

RN 690993-93-2 CAPLUS

CN 1H-Indole-6-carboxylic acid, 2-[2,3,5,6,8,9,12,13-octahydro-13-(2-methoxyethyl)-11H-1,4,7,10,13-benzotetraoxaazacyclopentadecin-16-yl]-, methyl ester (9CI) (CA INDEX NAME)

RN 690994-00-4 CAPLUS

CN 1H-Indole-6-carboxylic acid, 2-[13-[2-(dimethylamino)ethyl]2,3,5,6,8,9,12,13-octahydro-11H-1,4,7,10,13-benzotetraoxaazacyclopentadeci
n-16-yl]-, methyl ester (9CI) (CA INDEX NAME)

RN 690994-01-5 CAPLUS

CN 13H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-13-acetic acid, 16-(2,7-difluoro-6-hydroxy-3-oxo-3H-xanthen-9-yl)-2,3,5,6,8,9,11,12-octahydro-, monopotassium salt (9CI) (CA INDEX NAME)

● K

RN 846023-88-9 CAPLUS

CN 13H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-13-acetic acid, 2,3,5,6,8,9,11,12-octahydro-16-[6-(methoxycarbonyl)-1H-indol-2-yl]-, methyl ester (9CI) (CA INDEX NAME)

36080-56-5P 690993-63-6P 690993-64-7P 690993-65-8P 690993-66-9P 690993-70-5P 690993-71-6P 690993-72-7P 690993-73-8P 690993-74-9P 690993-84-1P 690993-85-2P 690993-87-4P 690993-88-5P 690993-89-6P 690993-92-1P 690993-94-3P 690993-95-4P

690993-96-5P 690993-97-6P 690993-98-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of crown ether derivs. as metal chelating agents or fluorescence indicators)

RN 36080-56-5 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 2,3,5,6,8,9,12,13-octahydro- (9CI) (CA INDEX NAME)

RN 690993-63-6 CAPLUS

CN 13H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-13-acetic acid, 2,3,5,6,8,9,11,12-octahydro-, methyl ester (9CI) (CA INDEX NAME)

RN 690993-64-7 CAPLUS

CN 13H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-13-acetic acid, 16-formyl-2,3,5,6,8,9,11,12-octahydro-, methyl ester (9CI) (CA INDEX NAME)

RN 690993-65-8 CAPLUS

CN 13H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-13-acetic acid, 16-(2,7-difluoro-3,6-dihydroxy-9H-xanthen-9-yl)-2,3,5,6,8,9,11,12-octahydro-, methyl ester (9CI) (CA INDEX NAME)

RN 690993-66-9 CAPLUS

CN 13H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-13-acetic acid, 16-(2,7-difluoro-6-hydroxy-3-oxo-3H-xanthen-9-yl)-2,3,5,6,8,9,11,12-octahydro-, methyl ester (9CI) (CA INDEX NAME)

RN 690993-70-5 CAPLUS

CN 13H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-13-acetic acid, 2,3,5,6,8,9,11,12-octahydro-16-[2-[4-(methoxycarbonyl)-2-nitrophenyl]ethenyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 690993-71-6 CAPLUS

CN 13H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-13-acetic acid, 2,3,5,6,8,9,11,12-octahydro-16-nitro-, methyl ester (9CI) (CA INDEX NAME)

RN 690993-72-7 CAPLUS

CN 13H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-13-acetic acid, 2,3,5,6,8,9,11,12-octahydro-16-[(4-sulfophenyl)azo]-, α-methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CH_2 - \stackrel{\circ}{U} - OMe \\ \hline \\ O & \\ O & \\ O & \\ \end{array}$$

RN 690993-73-8 CAPLUS

CN 13H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-13-acetic acid, 16-amino-2,3,5,6,8,9,11,12-octahydro-, methyl ester (9CI) (CA INDEX NAME)

RN 690993-74-9 CAPLUS

CN 13H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-13-carboxylic acid, 16-[[[3',6'-bis(acetyloxy)-2',7'-difluoro-3-oxospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-5-yl]carbonyl]amino]-2,3,5,6,8,9,11,12-octahydro-, methyl ester (9CI) (CA INDEX NAME)

RN 690993-84-1 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 2,3,5,6,8,9,12,13-octahydro-13-(methoxyacetyl)- (9CI) (CA INDEX NAME)

RN 690993-85-2 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 2,3,5,6,8,9,12,13-octahydro-13-(2-methoxyethyl)- (9CI) (CA INDEX NAME)

RN 690993-87-4 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-16-carboxaldehyde, 2,3,5,6,8,9,12,13-octahydro-13-(2-methoxyethyl)- (9CI) (CA INDEX NAME)

RN 690993-88-5 CAPLUS

ON 9H-Xanthene-3,6-diol, 2,7-difluoro-9-[2,3,5,6,8,9,12,13-octahydro-13-(2-methoxyethyl)-11H-1,4,7,10,13-benzotetraoxaazacyclopentadecin-16-yl]-(9CI) (CA INDEX NAME)

RN 690993-89-6 CAPLUS

CN 3H-Xanthen-3-one, 2,7-difluoro-6-hydroxy-9-[2,3,5,6,8,9,12,13-octahydro-13-(2-methoxyethyl)-11H-1,4,7,10,13-benzotetraoxaazacyclopentadecin-16-yl]-(9CI) (CA INDEX NAME)

RN 690993-92-1 CAPLUS

CN Benzoic acid, 3-nitro-4-[2-[2,3,5,6,8,9,12,13-octahydro-13-(2-methoxyethyl)-11H-1,4,7,10,13-benzotetraoxaazacyclopentadecin-16-yl]ethenyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 690993-94-3 CAPLUS

CN 13H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-13-acetic acid, 2,3,5,6,8,9,11,12-octahydro- α -oxo-, ethyl ester (9CI) (CA INDEX NAME)

RN 690993-95-4 CAPLUS

CN 13H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-13-acetamide, 2,3,5,6,8,9,11,12-octahydro-N,N-dimethyl- α -oxo- (9CI) (CA INDEX NAME)

RN 690993-96-5 CAPLUS

CN 13H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-13-ethanamine, 2,3,5,6,8,9,11,12-octahydro-N,N-dimethyl- (9CI) (CA INDEX NAME)

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-16-carboxaldehyde, 13-[2-(dimethylamino)ethyl]-2,3,5,6,8,9,12,13-octahydro- (9CI) (CA INDEX NAME)

RN 690993-98-7 CAPLUS

CN Benzoic acid, 4-[2-[13-[2-(dimethylamino)ethyl]-2,3,5,6,8,9,12,13-octahydro-11H-1,4,7,10,13-benzotetraoxaazacyclopentadecin-16-yl]ethenyl]-3-nitro-, methyl ester (9CI) (CA INDEX NAME)

$$CH_2-CH_2-NMe_2$$
 $CH=CH$
 CH
 CH

L5 ANSWER 3 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:892693 CAPLUS Full-text

DN 142:411333

TI Building up of macroring in the new synthesis of azacrown ethers. structure and complex formation of nitrobenzoazacrown ethers

AU Gromov, S. P.; Dmitrieva, S. N.; Churakova, M. V.; Vedernikov, A. I.; Kurchavov, N. A.; Kuzmina, L. G.; Kataeva, N. A.; Howard, J. A.

CS Photochemical Center, Russian Academy of Sciences, Moscow, 119421, Russia

SO Russian Journal of Organic Chemistry (Translation of Zhurnal Organicheskoi Khimii) (2004), 40(8), 1200-1209 CODEN: RJOCEQ; ISSN: 1070-4280

PB MAIK Nauka/Interperiodica Publishing

DT Journal

LA English

GΙ

$$N-Me$$
 $N-Me$
 $N-Me$

The preparation of aza crown ethers I [RX = bond, n = 0-2] by cyclization of I [R = H, X = I, n = 0-2] with various bases and in their absence was investigated. The nitrobenzoazacrown ethers obtained and their complexes with metal cations were studied by X-ray diffraction method and by 1H NMR titration I [RX = bond, n = 1] showed a capability to complex Ca2+ cation that significantly exceeded that of the nitrobenzocrown ether analog.

IT **511538-56-0P**

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and complexation of nitrobenzoazacrown ethers)

RN 511538-56-0 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 2,3,5,6,8,9,12,13-octahydro-13-methyl-16-nitro- (9CI) (CA INDEX NAME)

IT 511538-56-0DP, 2:1 complexes with lithium, calcium, and barium
850421-45-3P 850513-61-0P 850513-63-2P
850513-65-4P 850513-67-6P 850513-69-8P
850513-71-2P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and complexation of nitrobenzoazacrown ethers)

RN 511538-56-0 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 2,3,5,6,8,9,12,13-octahydro-13-methyl-16-nitro- (9CI) (CA INDEX NAME)

RN 850421-45-3 CAPLUS

CN Perchloric acid, ammonium salt, compd. with 2,3,5,6,8,9,12,13-octahydro-13-methyl-16-nitro-11H-1,4,7,10,13-benzotetraoxaazacyclopentadecine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 511538-56-0 CMF C15 H22 N2 O6

CM 2

CRN 7601-90-3 CMF Cl H O4

RN 850513-61-0 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

CM . 1

CRN 850513-60-9

CMF C15 H22 Li N2 O6

CCI CCS

CM 2

CRN 14797-73-0

CMF Cl O4

RN 850513-63-2 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

CM 1

CRN 850513-62-1

CMF C15 H22 N2 Na O6

CCI CCS

CM :

CRN 14797-73-0

CMF Cl O4

850513-65-4 CAPLUS RN CN INDEX NAME NOT YET ASSIGNED

> 1 CM

CRN

850513-64-3 C15 H22 K N2 O6 CMF

CCI CCS

CM

14797-73-0 CRN

Cl 04 CMF

850513-67-6 CAPLUS RN

INDEX NAME NOT YET ASSIGNED CN

> CM 1

CRN 850513-66-5

CMF C15 H22 Mg N2 O6

CCI . CCS

CM 2

CRN 14797~73-0 CMF Cl O4

0===0-

RN 850513-69-8 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

CM 1

CRN 850513-68-7

CMF C15 H22 Ca N2 O6

CCI CCS

CM 2

CRN 14797-73-0

CMF Cl O4

RN 850513-71-2 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

CM 1

CRN 850513-70-1

CMF C15 H22 Ba N2 O6

CCI CCS

CM 2

CRN 14797-73-0

CMF Cl O4

RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:414526 CAPLUS Full-text

DN 140:424969

TI Metal-complexing crown ether fluorescent indicators and their use with biological systems

IN Martin, Vladimir V.; Gee, Kyle

PA USA

SO U.S. Pat. Appl. Publ., 72 pp., Cont.-in-part of U.S. Ser. No. 26,302. CODEN: USXXCO

DT Patent

LA English

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PΙ	US 2004096978	A1	20040520	US 2003-634336 '	20030804	
	US 2002164616	A 1	20021107	US 2001-26302	20011219	
PRAI	US 2000-258266P	P	20001220			
	US 2001-26302	A2	20011219	•		

OS MARPAT 140:424969

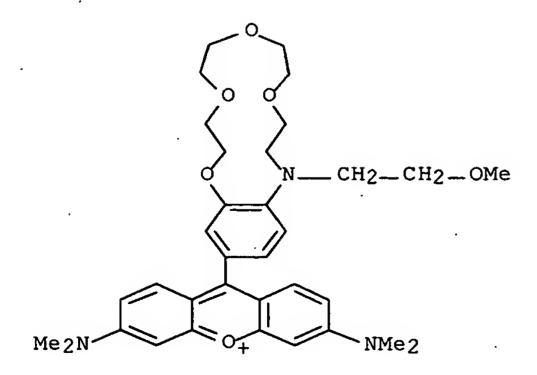
The invention discloses dibenzocrown ether chelators. These crown ethers are substituted by a dye moiety, a chemical reactive group, a conjugated substance, or a combination thereof. Chelators that are substituted by fluorescent dyes are particularly useful as indicators for metal cations, particularly Na + and K + ions, and particularly where binding of the target ion results in a change in the fluorescence properties of the indicator that can be correlated with the ion concentration Methods are provided for utilizing reactive groups on the chelators for conjugation to dyes, lipids, and polymers and methods for enhancing entry of the indicators into living cells.

IT 690993-91-0P 690993-93-2P 690994-00-4P 690994-01-5P 690994-05-9P 690994-07-1P 690994-08-2P 690994-09-3P 690994-10-6P 690994-11-7P 690994-12-8P 690994-13-9P 690994-14-0P

RL: IMF (Industrial manufacture); PREP (Preparation) (production of metal-complexing crown ether fluorescent indicators and their use with biol. systems)

RN 690993-91-0 CAPLUS

CN Xanthylium, 3,6-bis(dimethylamino)-9-[2,3,5,6,8,9,12,13-octahydro-13-(2-methoxyethyl)-11H-1,4,7,10,13-benzotetraoxaazacyclopentadecin-16-yl](9CI) (CA INDEX NAME)



RN 690993-93-2 CAPLUS

CN 1H-Indole-6-carboxylic acid, 2-[2,3,5,6,8,9,12,13-octahydro-13-(2-methoxyethyl)-11H-1,4,7,10,13-benzotetraoxaazacyclopentadecin-16-yl]-, methyl ester (9CI) (CA INDEX NAME)

RN 690994-00-4 CAPLUS

CN 1H-Indole-6-carboxylic acid, 2-[13-[2-(dimethylamino)ethyl]2,3,5,6,8,9,12,13-octahydro-11H-1,4,7,10,13-benzotetraoxaazacyclopentadeci
n-16-yl]-, methyl ester (9CI) (CA INDEX NAME)

RN 690994-01-5 CAPLUS

CN 13H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-13-acetic acid, 16-(2,7-difluoro-6-hydroxy-3-oxo-3H-xanthen-9-yl)-2,3,5,6,8,9,11,12-octahydro-, monopotassium salt (9CI) (CA INDEX NAME)

K

RN 690994-05-9 CAPLUS

CN 9H-Dibenzo[e,k][1,4,7,10,13]tetraoxaazacyclopentadecine-6,10(7H,11H)-dione, 17,18-dihydro-11-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 690994-07-1 CAPLUS

CN 9H-Dibenzo[e,k][1,4,7,10,13]tetraoxaazacyclopentadecine, 6,7,10,11,17,18-hexahydro-11-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 690994-08-2 CAPLUS

CN 9H-Dibenzo[e,k][1,4,7,10,13]tetraoxaazacyclopentadecine, 6,7,10,11,17,18-hexahydro- (9CI) (CA INDEX NAME)

RN 690994-09-3 CAPLUS

CN 11H-Dibenzo[e,k][1,4,7,10,13]tetraoxaazacyclopentadecine-11-acetic acid, 6,7,9,10,17,18-hexahydro-, methyl ester (9CI) (CA INDEX NAME)

RN 690994-10-6 CAPLUS

CN 11H-Dibenzo[e,k][1,4,7,10,13]tetraoxaazacyclopentadecine-11-acetic acid, 14-formyl-6,7,9,10,17,18-hexahydro-, methyl ester (9CI) (CA INDEX NAME)

RN 690994-11-7 CAPLUS

CN 11H-Dibenzo[e,k][1,4,7,10,13]tetraoxaazacyclopentadecine-11-acetic acid, 14-(2,7-difluoro-4a,9a-dihydro-3,6-dihydroxy-9H-xanthen-9-yl)-6,7,9,10,17,18-hexahydro-, methyl ester (9CI) (CA INDEX NAME)

RN 690994-12-8 CAPLUS

CN 11H-Dibenzo[e,k][1,4,7,10,13]tetraoxaazacyclopentadecine-11-acetic acid, 14-(2,7-difluoro-8a,10a-dihydro-6-hydroxy-3-oxo-3H-xanthen-9-yl)-6,7,9,10,17,18-hexahydro-, methyl ester (9CI) (CA INDEX NAME)

RN 690994-13-9 CAPLUS

CN 13H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-13-acetic acid, 16-(2,7-difluoro-6-hydroxy-3-oxo-3H-xanthen-9-yl)-2,3,5,6,8,9,11,12-octahydro- (9CI) (CA INDEX NAME)

RN 690994-14-0 CAPLUS

CN 2,5-Pyrrolidinedione, 1-[[[16-(2,7-difluoro-6-hydroxy-3-oxo-3H-xanthen-9-yl)-2,3,5,6,8,9,11,12-octahydro-13H-1,4,7,10,13-benzotetraoxaazacyclopentadecin-13-yl]acetyl]oxy]- (9CI) (CA INDEX NAME)

IT 36080-56-5P 690993-63-6P 690993-64-7P 690993-65-8P 690993-66-9P 690993-67-0P 690993-70-5P 690993-71-6P 690993-84-1P 690993-85-2P 690993-87-4P 690993-88-5P 690993-89-6P 690993-90-9P 690993-92-1P 690993-94-3P 690993-95-4P 690993-96-5P 690993-97-6P 690993-98-7P

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(production of metal-complexing crown ether fluorescent indicators and their use with biol. systems)

RN 36080-56-5 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 2,3,5,6,8,9,12,13-octahydro- (9CI) (CA INDEX NAME)

RN 690993-63-6 CAPLUS

CN 13H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-13-acetic acid, 2,3,5,6,8,9,11,12-octahydro-, methyl ester (9CI) (CA INDEX NAME)

RN 690993-64-7 CAPLUS

CN 13H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-13-acetic acid, 16-formyl-2,3,5,6,8,9,11,12-octahydro-, methyl ester (9CI) (CA INDEX NAME)

RN 690993-65-8 CAPLUS

CN 13H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-13-acetic acid, 16-(2,7-difluoro-3,6-dihydroxy-9H-xanthen-9-yl)-2,3,5,6,8,9,11,12-octahydro-, methyl ester (9CI) (CA INDEX NAME)

RN 690993-66-9 CAPLUS

CN 13H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-13-acetic acid, 16-(2,7-difluoro-6-hydroxy-3-oxo-3H-xanthen-9-yl)-2,3,5,6,8,9,11,12-octahydro-, methyl ester (9CI) (CA INDEX NAME)

RN 690993-67-0 CAPLUS

CN 13H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-13-acetic acid, 16-[6-[(acetyloxy)methoxy]-2,7-difluoro-3-oxo-3H-xanthen-9-yl]-2,3,5,6,8,9,11,12-octahydro-, methyl ester (9CI) (CA INDEX NAME)

RN 690993-70-5 CAPLUS

CN 13H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-13-acetic acid, 2,3,5,6,8,9,11,12-octahydro-16-[2-[4-(methoxycarbonyl)-2-nitrophenyl]ethenyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 690993-71-6 CAPLUS

CN 13H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-13-acetic acid, 2,3,5,6,8,9,11,12-octahydro-16-nitro-, methyl ester (9CI) (CA INDEX NAME)

RN 690993-84-1 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 2,3,5,6,8,9,12,13-octahydro-13-(methoxyacetyl)- (9CI) (CA INDEX NAME)

RN 690993-85-2 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 2,3,5,6,8,9,12,13-octahydro-13-(2-methoxyethyl)- (9CI) (CA INDEX NAME)

RN 690993-87-4 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-16-carboxaldehyde, 2,3,5,6,8,9,12,13-octahydro-13-(2-methoxyethyl)- (9CI) (CA INDEX NAME)

RN 690993-88-5 CAPLUS

CN 9H-Xanthene-3,6-diol, 2,7-difluoro-9-[2,3,5,6,8,9,12,13-octahydro-13-(2-methoxyethyl)-11H-1,4,7,10,13-benzotetraoxaazacyclopentadecin-16-yl]-(9CI) (CA INDEX NAME)

RN 690993-89-6 CAPLUS

CN 3H-Xanthen-3-one, 2,7-difluoro-6-hydroxy-9-[2,3,5,6,8,9,12,13-octahydro-13-(2-methoxyethyl)-11H-1,4,7,10,13-benzotetraoxaazacyclopentadecin-16-yl]-(9CI) (CA INDEX NAME)

RN 690993-90-9 CAPLUS

CN 3H-Xanthen-3-one, 6-[(acetyloxy)methoxy]-2,7-difluoro-9-[2,3,5,6,8,9,12,13-octahydro-13-(2-methoxyethyl)-11H-1,4,7,10,13-

benzotetraoxaazacyclopentadecin-16-yl]- (9CI) (CA INDEX NAME)

RN 690993-92-1 CAPLUS

CN Benzoic acid, 3-nitro-4-[2-[2,3,5,6,8,9,12,13-octahydro-13-(2-methoxyethyl)-11H-1,4,7,10,13-benzotetraoxaazacyclopentadecin-16-yl]ethenyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 690993-94-3 CAPLUS

CN 13H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-13-acetic acid, 2,3,5,6,8,9,11,12-octahydro- α -oxo-, ethyl ester (9CI) (CA INDEX NAME)

RN 690993-95-4 CAPLUS

CN 13H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-13-acetamide, 2,3,5,6,8,9,11,12-octahydro-N,N-dimethyl- α -oxo- (9CI) (CA INDEX NAME)

RN 690993-96-5 CAPLUS

CN 13H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-13-ethanamine, 2,3,5,6,8,9,11,12-octahydro-N,N-dimethyl- (9CI) (CA INDEX NAME)

RN 690993-97-6 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-16-carboxaldehyde, 13-[2-(dimethylamino)ethyl]-2,3,5,6,8,9,12,13-octahydro- (9CI) (CA INDEX NAME)

RN 690993-98-7 CAPLUS

CN Benzoic acid, 4-[2-[13-[2-(dimethylamino)ethyl]-2,3,5,6,8,9,12,13-octahydro-11H-1,4,7,10,13-benzotetraoxaazacyclopentadecin-16-yl]ethenyl]-3-nitro-, methyl ester (9CI) (CA INDEX NAME)

IT 690993-68-1P 690993-69-2P 690993-72-7P 690993-73-8P 690993-74-9P

RL: IMF (Industrial manufacture); TEM (Technical or engineered material

use); PREP (Preparation); USES (Uses)
 (production of metal-complexing crown ether fluorescent indicators and
 their use with biol. systems)

RN 690993-68-1 CAPLUS

CN Xanthylium, 3,6-bis(dimethylamino)-9-[2,3,5,6,8,9,12,13-octahydro-13-(2-methoxy-2-oxoethyl)-11H-1,4,7,10,13-benzotetraoxaazacyclopentadecin-16-yl]-(9CI) (CA INDEX NAME)

RN 690993-69-2 CAPLUS

CN Boron, difluoro[methyl 16-[(3,5-dimethyl-1H-pyrrol-2-yl-κN)(3,5-dimethyl-2H-pyrrol-2-ylidene-κN)methyl]-2,3,5,6,8,9,11,12-octahydro-13H-1,4,7,10,13-benzotetraoxaazacyclopentadecine-13-acetato]-, (T-4)-(9CI) (CA INDEX NAME)

RN 690993-72-7 CAPLUS

CN 13H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-13-acetic acid, 2,3,5,6,8,9,11,12-octahydro-16-[(4-sulfophenyl)azo]-, α -methyl ester (9CI) (CA INDEX NAME)

$$CH_2-C-OMe$$
 $N=N$
 $SO3H$

RN 690993-73-8 CAPLUS

CN 13H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-13-acetic acid, 16-amino-2,3,5,6,8,9,11,12-octahydro-, methyl ester (9CI) (CA INDEX NAME)

RN 690993-74-9 CAPLUS

CN 13H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-13-carboxylic acid,
16-[[[3',6'-bis(acetyloxy)-2',7'-difluoro-3-oxospiro[isobenzofuran1(3H),9'-[9H]xanthen]-5-yl]carbonyl]amino]-2,3,5,6,8,9,11,12-octahydro-,
methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{AcO} \\ \text{F} \\ \\ \text{CH}_2\text{-C-OMe} \\ \end{array}$$

L5 ANSWER 5 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

.AN 2004:337986 CAPLUS Full-text

DN 141:173682

TI DFT calculation of benzoazacrown ethers and their complexes with calcium perchlorate

AU Avakyan, V. G.; Gromov, S. P.; Vedernikov, A. I.; Dmitrieva, S. N.; Alfimov, M. V.

CS Center of Photochemistry of the Russian Academy of Sciences, Moscow, 119421, Russia

SO Russian Chemical Bulletin (Translation of Izvestiya Akademii Nauk, Seriya Khimicheskaya) (2004), 53(1), 24-32 CODEN: RCBUEY; ISSN: 1066-5285

PB Kluwer Academic/Consultants Bureau

DT Journal

LA English

AB The complexation consts. of several azacrown ethers with Ca(ClO4)2 were determined and turned out to be the higher, the large the macrocycle. The structures of free ligands and their complexes and the complexation energies were calculated by the DFT method. In the aza-12(15)-crown-4(5) ether complexes with Ca(ClO4)2, the metal cations lie outside the averaged plane of heteroatoms of the macrocycle, and the coordination of both counterions is Vlike. In the complexes of aza-18-crown-6 ethers, the counterions are in the axial position relatively to the macrocycle in the center of which the Ca2+ ion is localized. The complexation energies increase with an increase in the size of the azacrown ether macrocycle. The involvement of the nitrogen atom in binding with the Ca2+ ion decreases with the expansion of the macrocycle. Two methods for quant. estimation of the degree of pre-organization of ligands to complexation were considered: geometric and energetic methods. Benzoaza-15crown-5 ether is a ligand which is more pre-organized to complexation than Nphenylaza-15-crown-5 ether.

IT 247074-86-8 247074-88-0 733767-60-7 733767-63-0 733767-67-4 733767-70-9

RL: PRP (Properties)

(DFT calcn. on benzoazacrown ethers and their complexes with calcium perchlorate)

RN 247074-86-8 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-16-carboxaldehyde, 2,3,5,6,8,9,12,13-octahydro-13-methyl- (9CI) (CA INDEX NAME)

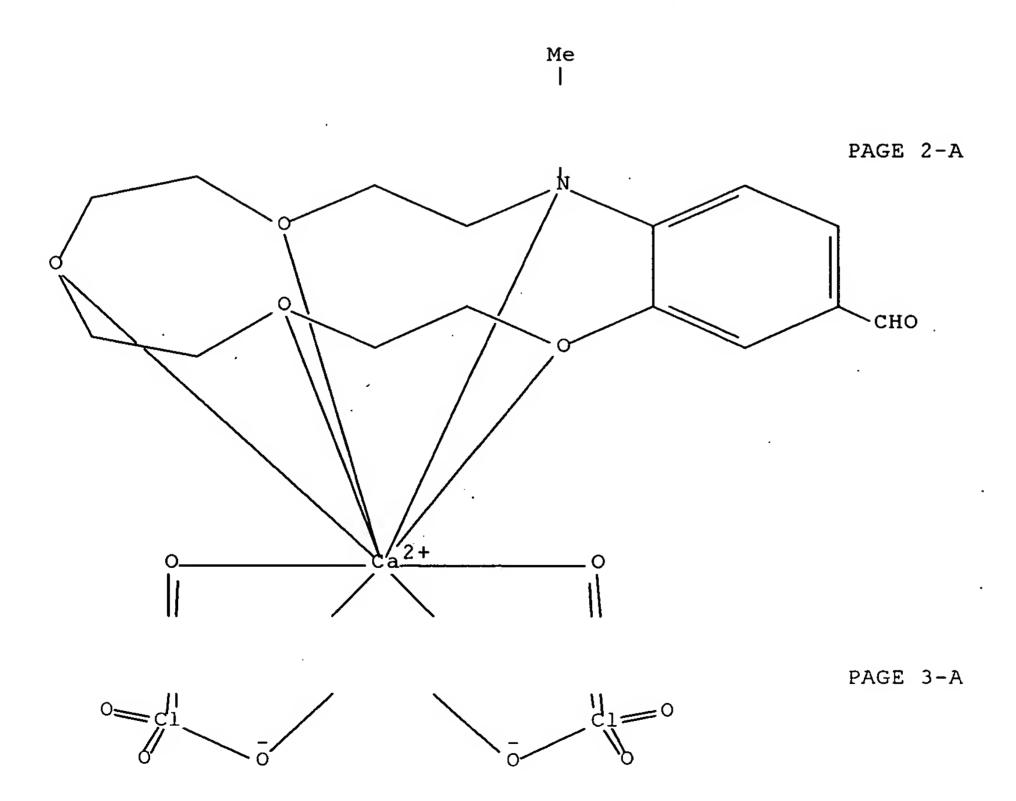
RN 247074-88-0 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-16-carboxaldehyde, 2,3,5,6,8,9,12,13-octahydro- (9CI) (CA INDEX NAME)

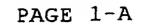
RN 733767-60-7 CAPLUS

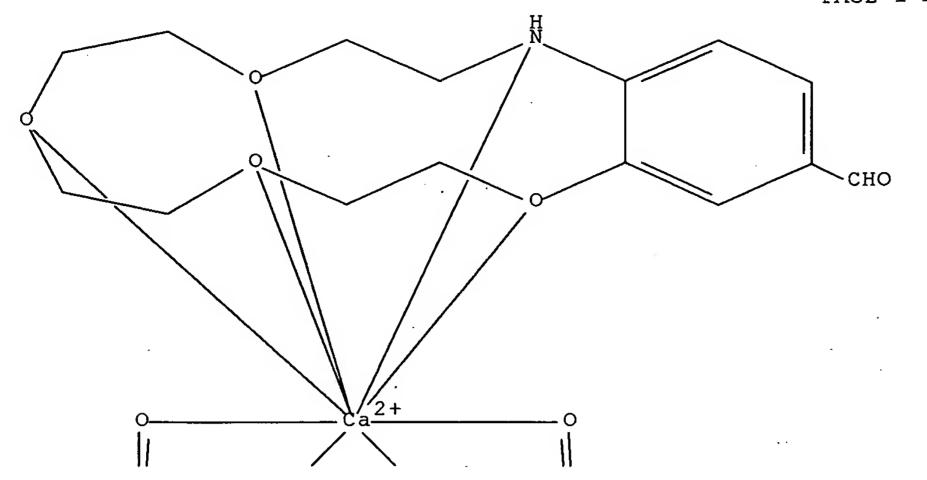
CN Calcium, (2,3,5,6,8,9,12,13-octahydro-13-methyl-11H-1,4,7,10,13-benzotetraoxaazacyclopentadecine-16-carboxaldehydeκN13,κO1,κO4,κO7,κO10)bis(perchloratoκO,κO')- (9CI) (CA INDEX NAME)

PAGE 1-A



RN 733767-63-0 CAPLUS
CN Calcium, (2,3,5,6,8,9,12,13-octahydro-11H-1,4,7,10,13-benzotetraoxaazacyclopentadecine-16-carboxaldehydeκN13,κΟ1,κΟ4,κΟ7,κΟ10)bis(perchloratoκΟ,κΟ')- (9CI) (CA INDEX NAME)





PAGE 2-A

RN 733767-67-4 CAPLUS

CN Calcium(1+), (2,3,5,6,8,9,12,13-octahydro-13-methyl-11H-1,4,7,10,13-benzotetraoxaazacyclopentadecine-16-carboxaldehydeκN13,κΟ1,κΟ4,κΟ7,κΟ10) (perchloratoκΟ,κΟ')- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 733767-70-9 CAPLUS

CN Calcium(1+), (2,3,5,6,8,9,12,13-octahydro-11H-1,4,7,10,13-benzotetraoxaazacyclopentadecine-16-carboxaldehyde- κ N13, κ O1, κ O4, κ O7, κ O10) (perchlorato- κ O, κ O')- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 6 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2003:936890 CAPLUS Full-text

DN 141:23560

TI A preparation of benzoazacrown ether derivatives from benzocrown ether derivatives

IN Gromov, S. P.; Dmitrieva, S. N.; Churakova, M. V.

PA Russia

SO Russ., No pp. given CODEN: RUXXE7

DT Patent

LA Russian

FAN.CNT 1

1	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
-							
PI I	RU 2215738 .	C1	20031110	RU 2002-118852	20020717		
PRAI I	RU 2002-118852		20020717				
OS I	MARPAT 141:23560						
GT							

Ι

II

The invention relates to novel nitro-derivs. of N-alkylbenzoazacrown ether of formula I [wherein: R is alkyl; X = N; n = 1-4]. These compds. can be used as selective reagents for cations of ammonium, alkaline or alkaline-earth metals. The stability consts. of I [R is alkyl; X = N; n = 1-4] with NaClO4, NH4ClO4, Mg(ClO4)2, Ba(ClO4)2, and Ca(ClO4)2 were determined For instance, compound I (R = Me, X = N, n = 1) was prepared via amination/ring opening of I (no R, X = O, n = 1) by methylamine (example 1), chlorination of the obtained II (Y = OH) by SOCl2 (example 4), iodination of the obtained II (Y = Cl, example 7), and subsequent cyclization (example 10).

IT **511538-56-0P**

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of nitro-derivs. of n-alkylbenzoazacrown ether from derivs. of nitrobenzocrown ether)

RN 511538-56-0 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 2,3,5,6,8,9,12,13-octahydro-13-methyl-16-nitro- (9CI) (CA INDEX NAME)

L5 ANSWER 7 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2003:692254 CAPLUS Full-text

DN 139:323504

TI Novel promising benzoazacrown ethers as a result of ring transformation of benzocrown ethers: synthesis, structure, and complexation with Ca2+

AU Gromov, Sergey P.; Dmitrieva, Svetlana N.; Vedernikov, Artem I.; Kuz'mina, Lyudmila G.; Churakov, Andrey V.; Strelenko, Yuri A.; Howard, Judith A. K.

CS Photochemistry Center of the Russian Academy of Sciences, Moscow, 119421, Russia

SO European Journal of Organic Chemistry (2003), (16), 3189-3199 CODEN: EJOCFK; ISSN: 1434-193X

PB Wiley-VCH Verlag GmbH & Co. KGaA

DT Journal

LA English

OS CASREACT 139:323504

GI

$$O = CH \xrightarrow{NR} O \xrightarrow{O} O$$

As series of promising benzoazacrown ethers with the nitrogen atom conjugated with the benzene ring, i.e., I (R = Me, H; n = 0, 1, 2), were synthesized using a novel procedure based on stepwise transformation of the macroheterocycle. The structures and spectral properties of I and their complexes with Ca2+ were studied by X-ray diffraction and 1H, 13C, and 15N NMR spectroscopy including the 2D NOESY technique.

IT 247074-88-0P

RL: BYP (Byproduct); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and structure of benzoazacrown ether aldehydes and their complexation with calcium ion)

RN 247074-88-0 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-16-carboxaldehyde, 2,3,5,6,8,9,12,13-octahydro- (9CI) (CA INDEX NAME)

IT 247074-86-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and structure of benzoazacrown ether aldehydes and their complexation with calcium ion)

RN 247074-86-8 CAPLUS

CN 11H-1, 4, 7, 10, 13-Benzotetraoxaazacyclopentadecine-16-carboxaldehyde,

IT 615286-92-5P 615286-95-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and structure of benzoazacrown ether aldehydes and their complexation with calcium ion)

RN 615286-92-5 CAPLUS

CN Calcium(2+), $(2,3,5,6,8,9,12,13-\text{octahydro}-13-\text{methyl}-11H-1,4,7,10,13-\text{benzotetraoxaazacyclopentadecine}-<math>\kappa$ N13, κ O1, κ O4, κ O7, κ O10)- (9CI) (CA INDEX NAME)

RN 615286-95-8 CAPLUS
CN Calcium(2+), (2,3,5,6,8,9,12,13-octahydro-11H-1,4,7,10,13-benzotetraoxaazacyclopentadecine-κN13,κO1,κO4,κO7,κO10)- (9CI) (CA INDEX NAME)

RE.CNT 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 8 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2003:326945 CAPLUS Full-text

DN 139:62064

TI Coordination Properties of a Diarylaza Crown Ether Appended with a Luminescent [Ru(bipy)3]2+ Unit

AU Charbonniere, Loiec J.; Ziessel, Raymond F.; Sams, Craig A.; Harriman, Anthony

CS Laboratoire de Chimie Moleculaire UMR 7008 au CNRS, Ecole de Chimie Polymere et Materiaux, Strasbourg, 67087, Fr.

SO Inorganic Chemistry (2003), 42(11), 3466-3474 CODEN: INOCAJ; ISSN: 0020-1669

PB American Chemical Society

DT Journal

LA English

OS CASREACT 139:62064

GI

The [Ru(bipy)2(1)](PF6)2 (bipy refers to 2,2'-bipyridine) complex, comprising a Ru(II) tris(2,2'-bipyridine) luminophor covalently linked to a di[(o-triethyleneglycoxy)phenyl]amine crown ether (1 = I), was synthesized and fully characterized. The photophys. properties of this metal complex were examined in solution at ambient temperature Luminescence from the metal complex is enhanced significantly in the presence of various adventitious cations, including protons. In particular, Li+ cations bind to the crown ether, as evidenced by 1H NMR and luminescence spectroscopy. Cation binding serves to decrease the rate of reductive quenching of the triplet state of the metal complex, thereby increasing the extent of luminescence. The solution-phase conformation of [Ru(bipy)2(1)](PF6)2, with and without encapsulated Li+, was examined by 2-dimensional NMR and by mol. dynamics simulations.

IT 548491-25-4 548491-26-5 548491-27-6

RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); FORM (Formation, nonpreparative); PROC (Process)

(elec. potential of couple containing)

RN 548491-25-4 CAPLUS

CN Ruthenium(1+), bis(2,2'-bipyridine-κN1,κN1')[6,7,9,10,12,13-hexahydro-19-[(5'-methyl[2,2'-bipyridin]-5-yl-κN1,κN1')methyl]19H-dibenzo[k,n][1,4,7,10,13]tetraoxaazacyclopentadecine]-, (OC-6-33)(9CI) (CA INDEX NAME)

RN 548491-26-5 CAPLUS

CN Ruthenium, bis(2,2'-bipyridine-κN1,κN1')[6,7,9,10,12,13-hexahydro-19-[(5'-methyl[2,2'-bipyridin]-5-yl-κN1,κN1')methyl]-19H-dibenzo[k,n][1,4,7,10,13]tetraoxaazacyclopentadecine]-, (OC-6-33)-(9CI) (CA INDEX NAME)

RN 548491-27-6 CAPLUS

CN Ruthenate(1-), bis(2,2'-bipyridine-κN1,κN1')[6,7,9,10,12,13-hexahydro-19-[(5'-methyl[2,2'-bipyridin]-5-yl-κN1,κN1')methyl]-19H-dibenzo[k,n][1,4,7,10,13]tetraoxaazacyclopentadecine]-, (OC-6-33)-(9CI) (CA INDEX NAME)

IT 548491-24-3

RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative) (formation of in preparation of diarylaza crown ether appended bipyridine)

RN 548491-24-3 CAPLUS

CN 19H-Dibenzo[k,n][1,4,7,10,13]tetraoxaazacyclopentadecinium, 6,7,9,10,12,13-hexahydro-19,19-bis[(5'-methyl[2,2'-bipyridin]-5-yl)methyl]-(9CI) (CA INDEX NAME)

IT 281680-54-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and complexation with ruthenium)

RN 281680-54-4 CAPLUS

CN 19H-Dibenzo[k,n][1,4,7,10,13]tetraoxaazacyclopentadecine, 6,7,9,10,12,13-hexahydro-19-[(5'-methyl[2,2'-bipyridin]-5-yl)methyl]-(9CI) (CA INDEX NAME)

IT 548491-22-1DP, alkali metal complexes

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and triplet lifetime)

RN 548491-22-1 CAPLUS

CN Ruthenium(2+), bis(2,2'-bipyridine-κN1,κN1')[6,7,9,10,12,13-hexahydro-19-[(5'-methyl[2,2'-bipyridin]-5-yl-κN1,κN1')methyl]19H-dibenzo[k,n][1,4,7,10,13]tetraoxaazacyclopentadecine]-, (OC-6-33)(9CI) (CA INDEX NAME)

IT 548491-28-7P

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

(preparation, cyclic voltammetry, calculated mol. structure from mol. dynamics

simulations and luminescence)

RN 548491-28-7 CAPLUS

CN Ruthenium(2+), bis(2,2'-bipyridine-κN1,κN1')[6,7,9,10,12,13-hexahydro-19-[(5'-methyl[2,2'-bipyridin]-5-yl-κN1,κN1')methyl]-19H-dibenzo[k,n][1,4,7,10,13]tetraoxaazacyclopentadecine]-, conjugate monoacid, (OC-6-33)- (9CI) (CA INDEX NAME)

IT 281680-51-1P

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

(preparation, cyclic voltammetry, luminescence quenching of ruthenium diarylaza crown ether appended bipyridine complex with and reaction with 5-bromomethyl-5'-methyl-2,2'-bipyridine)

RN 281680-51-1 CAPLUS

CN 19H-Dibenzo[k,n][1,4,7,10,13]tetraoxaazacyclopentadecine, 6,7,9,10,12,13-hexahydro- (9CI) (CA INDEX NAME)

IT 548491-23-2P

RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

(preparation, luminescence, cyclic voltammetry, quenching from alkali metals

encapsulation and mol. structure from mol. dynamics simulations)

RN 548491-23-2 CAPLUS

CN Ruthenium(2+), bis(2,2'-bipyridine-κN1,κN1')[6,7,9,10,12,13-hexahydro-19-[(5'-methyl[2,2'-bipyridin]-5-yl-κN1,κN1')methyl]-19H-dibenzo[k,n][1,4,7,10,13]tetraoxaazacyclopentadecine]-, (OC-6-33)-, bis[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

CM 1

CRN 548491-22-1

CMF C50 H47 N7 O4 Ru

CCI CCS

CM 2

CRN 16919-18-9

CMF F6 P

CCI CCS

RE.CNT '41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 9 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2003:244251 CAPLUS Full-text

DN 139:133548

TI A novel ring transformation of nitrobenzocrown ethers as a route to nitrobenzoazacrown compounds

AU Gromov, Sergei P.; Dmitrieva, Svetlana N.; Churakova, Marina V.

CS Photochem. Center, RAS, Moscow, Russia

SO Synthesis (2003), (4), 593-597 CODEN: SYNTBF; ISSN: 0039-7881

PB Georg Thieme Verlag

DT Journal

LA English

OS CASREACT 139:133548

AB A method for the synthesis of previously unknown nitro derivs. of benzoazacrown compds. in which nitrogen is conjugated with the benzene ring, based on readily available benzocrown ethers used as synthons, was developed. This approach can serve as a useful tool in the synthesis of diverse benzoazacrown derivs.

IT 511538-56-0P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of nitrobenzoazacrown compds. by ring transformation of nitrobenzocrown ethers)

RN 511538-56-0 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 2,3,5,6,8,9,12,13-octahydro-13-methyl-16-nitro- (9CI) (CA INDEX NAME)

RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L5 ANSWER 10 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN
- AN 2002:836585 CAPLUS Full-text
- DN 138:321259
- TI Synthesis of nitrobenzoazacrown compounds by ring transformations of nitrobenzo crown ethers
- AU Gromov, S. P.; Dmitrieva, S. N.; Churakova, M. V.; Turchanov, A. Yu.
- CS Center of Photochemistry, Russian Academy of Sciences, Moscow, 117421, Russia
- SO Russian Chemical Bulletin (Translation of Izvestiya Akademii Nauk, Seriya Khimicheskaya) (2002), 51(7), 1335-1336 CODEN: RCBUEY; ISSN: 1066-5285
- PB Kluwer Academic/Consultants Bureau
- DT Journal
- LA English
- OS CASREACT 138:321259
- AB A stepwise synthetic approach for preparation of a series of nitrobenzoazacrowns via cyclization of corresponding podands was proposed. The yield of the final compds. was 36-80%.
- IT 511538-56-0P
 - RL: SPN (Synthetic preparation); PREP (Preparation) (stepwise preparation of nitrobenzoazacrown compds. by ring transformations of corresponding nitrobenzo crown ether podands)
- RN 511538-56-0 CAPLUS
- CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 2,3,5,6,8,9,12,13-octahydro-13-methyl-16-nitro- (9CI) (CA INDEX NAME)

RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 11 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2002:287594 CAPLUS Full-text

DN 137:24811

TI Substitution Effect, Absorption, and Fluorescence Behaviors of 11,12-Benzo-1,7,10,13-tetraoxa-4-aza- cyclopentadec-11-ene (Benzoaza-15-crown-5) Derivatives upon Cation Complexation in Solvent Extraction

AU Nakamura, Mitsunobu; Yokono, Hideaki; Tomita, Ken-ichi; Ouchi, Mikio; Miki, Masamichi; Dohno, Reizo

CS Department of Engineering Science and Department of Applied Chemistry, Himeji Institute of Technology, Himeji, Hyogo, 671-2201, Japan

SO Journal of Organic Chemistry (2002), 67(10), 3533-3536 CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

DT Journal

LA English

AB Substitution effect, absorption, and fluorescence behaviors of some benzoaza15-crown-5 derivs. upon cation complexation in solvent extraction were
studied. The introduction of a substituent on the nitrogen atom in benzoaza15-crown-5 enhanced extractabilities in the solvent extraction of aqueous
alkali metal picrates. The nondonating substituents raised the cation
selectivity for Na+ over K+, but the donating substituents reduced the cation
selectivity. The absorption and fluorescence spectral behavior was different
with the alkali metal cations.

IT **36080-56-5P**, Benzoaza-15-crown-5

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

(substituent effect on alkali metal solvent extraction/complexation by benzoaza-15-crown-5 N-derivs.)

RN 36080-56-5 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 2,3,5,6,8,9,12,13-octahydro- (9CI) (CA INDEX NAME)

RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 12 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2000:282640 CAPLUS Full-text

DN 133:89509

TI Cyclic di[(o-polyethyleneglycoxy)phenyl]amine: new members in the crown ether family

AU Charbonniere, Loic J.; Ziessel, Raymond F.

CS Laboratoire de Chimie, d'Electronique et de Photonique Moleculaires, associe au CNRS, Ecole Chimie, Polymeres, Materiaux (ECPM), Strasbourg, 67087, Fr.

SO Tetrahedron Letters (2000), 41(14), 2373-2376 CODEN: TELEAY; ISSN: 0040-4039

PB Elsevier Science Ltd.

DT Journal

LA English

The synthesis of cyclic ethers based on polyethylene glycol chains grafted on di(o-hydroxyphenyl)amine is described. The starting (2-HOC6H4)2NH was obtained from a melted salt procedure and coupled to the tosylated tri-, tetra- and pentaethylene glycol. The X-ray crystal structure of the tetraethylene glycol derivative was determined For the triethylene glycol compound, alkylation of the nitrogen atom with 5-bromomethyl-5'-methyl-2,2'-bipyridine (excess or 1 equivalent) led either to the quaternary ammonium salt or to the tertiary amine derivs., resp. The latter reacted with [Re(CO)5Cl] to give the corresponding Re(I) complex in a facial configuration.

IT 281680-51-1P 281680-54-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reactions of cyclic di[(ooligoethyleneglycoxy)phenyl]amine

s)

RN 281680-51-1 CAPLUS

CN 19H-Dibenzo[k,n][1,4,7,10,13]tetraoxaazacyclopentadecine, 6,7,9,10,12,13-hexahydro- (9CI) (CA INDEX NAME)

RN 281680-54-4 CAPLUS

CN 19H-Dibenzo[k,n][1,4,7,10,13]tetraoxaazacyclopentadecine, 6,7,9,10,12,13-hexahydro-19-[(5'-methyl[2,2'-bipyridin]-5-yl)methyl]-(9CI) (CA INDEX NAME)

IT 281680-55-5P 282109-76-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and reactions of cyclic di[(o-oligoethyleneglycoxy)phenyl]amine s)

RN 281680-55-5 CAPLUS

CN 19H-Dibenzo[k,n][1,4,7,10,13]tetraoxaazacyclopentadecinium, 6,7,9,10,12,13-hexahydro-19,19-bis[(5'-methyl[2,2'-bipyridin]-5-yl)methyl]-, bromide (9CI) (CA INDEX NAME)

RN 282109-76-6 CAPLUS

CN Rhenium, tricarbonylchloro[6,7,9,10,12,13-hexahydro-19-[(5'-methyl[2,2'-bipyridin]-5-yl-κN1,κN1')methyl]-19H-dibenzo[k,n][1,4,7,10,13]tetraoxaazacyclopentadecine]- (9CI) (CA INDEX NAME)

RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 13 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2000:117460 CAPLUS Full-text

DN 132:265278

TI Synthesis and Characterization of a Chiral, Aza-15-Crown-5-Functionalized Ferrocenyldiphosphine Ligand for Asymmetric Catalysis

AU Landis, Clark R.; Sawyer, Rachel A.; Somsook, Ekasith

CS Department of Chemistry, University of Wisconsin-Madison, Madison, WI, 53705, USA

SO Organometallics (2000), 19(6), 994-1002 CODEN: ORGND7; ISSN: 0276-7333

PB American Chemical Society

DT Journal

LA English

OS CASREACT 132:265278

GI

AB A chiral ferrocenyldiphosphine ligand that is functionalized with an aza crown ether, (S)-1-[(R)-1',2-bis(diphenylphosphino)ferrocenyl]ethyl-1-aza-2,3-benzo-15-crown-5 (1; shown as I), was synthesized. Both the resolved and racemic ligands react rapidly with Pt(II) precursors to form stable metalligand adducts; the complexes PtMeI(rac-1) and PtMe2(rac-1) were characterized crystallog. Reaction of rac-1 with [Rh(NBD)2]OTf yields [Rh(NBD)(rac-1)]OTf. The three-dimensional solution structure of [Rh(NBD)(rac-1)]OTf was determined by NOESY expts. and anal. using the two-dimensional conformer population anal. algorithm (2DCPA). The NOESY data reveal a rapid, pairwise chemical exchange between vinyl protons. [Rh(NBD)(rac-1)]OTf is a catalyst precursor for hydrogenation reactions. However, the lability of the aza crown ether may limit the ability of these catalysts to control selectivity via secondary interactions.

IT **263026-95-5P**, 1-Aza-2,3-benzo-15-crown-5 triflate

RL: SPN (Synthetic preparation); PREP (Preparation)

(formation from aza-15-crown-5-functionalized ferrocenyldiphosphine and allylammonium triflate)

RN 263026-95-5 CAPLUS

CN Methanesulfonic acid, trifluoro-, compd. with 2,3,5,6,8,9,12,13-octahydro-11H-1,4,7,10,13-benzotetraoxaazacyclopentadecine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 36080-56-5

CM 2

CRN 1493-13-6 CMF C H F3 O3 S

IT 263026-92-2P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and 2DCPA conformational anal. of)

RN 263026-92-2 CAPLUS

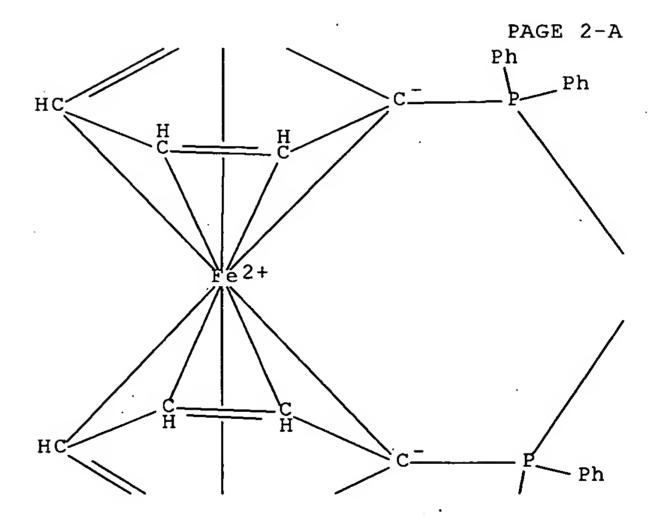
CN Rhodium(1+), $[(2,3,5,6-\eta)-bicyclo[2.2.1]hepta-2,5-diene][rel-(1R)-1,1'-bis(diphenylphosphino-<math>\kappa P$)-2-[(1R)-1-(2,3,5,6,8,9,11,12-octahydro-13H-1,4,7,10,13-benzotetraoxaazacyclopentadecin-13-yl)ethyl]ferrocene]-, stereoisomer, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

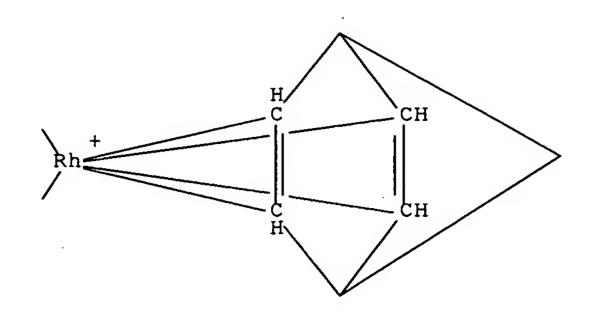
CM 1

CRN 263026-91-1

. CMF $C57\ H59\ Fe\ N\ O4\ P2\ Rh$

CCI CCS





PAGE 3-A Ph

CM 2

CRN 37181-39-8 CMF C F3 O3 S

IT 36080-56-5P, 1-Aza-2, 3-benzo-15-crown-5

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and N-functionalization by (phosphinoferrocenyl)ethyl)

RN 36080-56-5 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 2,3,5,6,8,9,12,13-octahydro- (9CI) (CA INDEX NAME)

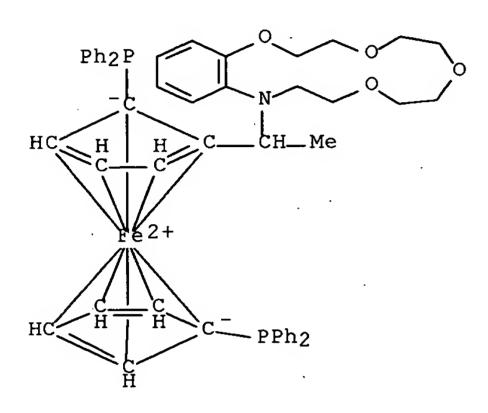
IT 263026-88-6P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(preparation and catalysis of asym. hydrogenation of Me $\alpha\text{-}$ acetamidocinnamate by rhodium complex and)

RN 263026-88-6 CAPLUS

CN Ferrocene, 1,1'-bis(diphenylphosphino)-2-[(1S)-1-(2,3,5,6,8,9,11,12-octahydro-13H-1,4,7,10,13-benzotetraoxaazacyclopentadecin-13-yl)ethyl]-, (1S)- (9CI) (CA INDEX NAME)



IT 263026-89-7P 263026-93-3P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal structure of)

RN 263026-89-7 CAPLUS

CN Platinum, [rel-(1R)-1,1'-bis(diphenylphosphino-κP)-2-[(1R)-1-(2,3,5,6,8,9,11,12-octahydro-13H-1,4,7,10,13-benzotetraoxaazacyclopentadecin-13-yl)ethyl]ferrocene]dimethyl-, (SP-4-3)- (9CI) (CA INDEX NAME)

сн-ме

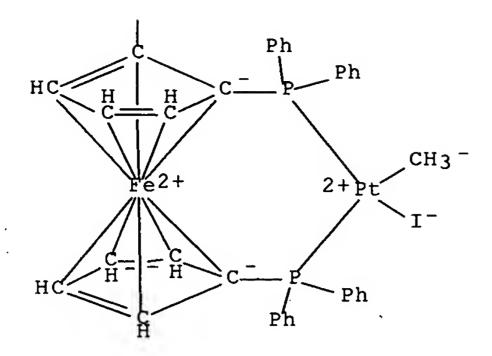
PAGE 1-A

HC
$$\frac{H}{C}$$
 $\frac{C}{C}$ $\frac{Ph}{C}$ $\frac{Ph}{C}$ $\frac{CH_3}{CH_3}$ $\frac{CH_3}{CH_3}$

RN 263026-93-3 CAPLUS

CN Platinum, [rel-(1R)-1,1'-bis(diphenylphosphino-κP)-2-[(1R)-1-(2,3,5,6,8,9,11,12-octahydro-13H-1,4,7,10,13-benzotetraoxaazacyclopentadecin-13-yl)ethyl]ferrocene]iodomethyl-, (SP-4-2)- (9CI) (CA INDEX NAME)

PAGE 1-A



IT 263026-90-0P 263389-56-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 263026-90-0 CAPLUS

CN Platinum, [rel-(lR)-1,1'-bis(diphenylphosphino-κP)-2-[(lR)-1-(2,3,5,6,8,9,11,12-octahydro-13H-1,4,7,10,13-benzotetraoxaazacyclopentadecin-13-yl)ethyl]ferrocene]dichloro-, (SP-4-3)- (9CI) (CA INDEX NAME)

PAGE 1-A

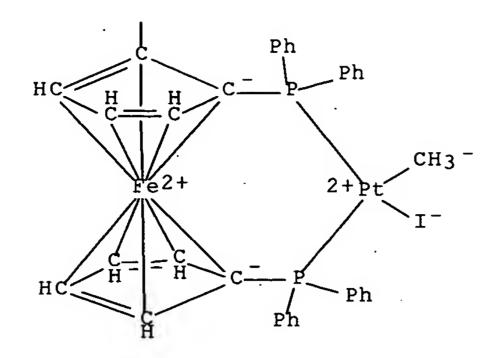
HC H C Ph
$$C^{-}$$
 Ph C^{-} Ph

RN 263389-56-6 CAPLUS

CN Platinum, [rel-(1R)-1,1'-bis(diphenylphosphino-κP)-2-[(1R)-1-(2,3,5,6,8,9,11,12-octahydro-13H-1,4,7,10,13-benzotetraoxaazacyclopentadecin-13-yl)ethyl]ferrocene]iodomethyl-, (SP-4-3)- (9CI) (CA INDEX NAME)

PAGE 1-A

--



IT 263389-57-7P

RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation, coordinative substitutions with platinum and rhodium complexes

and catalysis of asym. hydrogenation of Me $\alpha\text{--acetamidocinnamate}$ by rhodium complex and)

RN 263389-57-7 CAPLUS

CN Ferrocene, 1,1'-bis(diphenylphosphino)-2-[(1R)-1-(2,3,5,6,8,9,11,12-octahydro-13H-1,4,7,10,13-benzotetraoxaazacyclopentadecin-13-yl)ethyl]-, (1R)-rel-(9CI) (CA INDEX NAME)

RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 14 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1999:560743 CAPLUS Full-text

DN 131:299435

TI New approach to the synthesis of benzoazacrown ethers

AU Gromov, S. P.; Vedernikov, A. I.; Dmitrieva, S. N.

CS Photochemistry Center, Russian Academy of Sciences, Moscow, 117421, Russia

SO Russian Chemical Bulletin (Translation of Izvestiya Akademii Nauk, Seriya Khimicheskaya) (1999), 48(6), 1190-1192

CODEN: RCBUEY; ISSN: 1066-5285

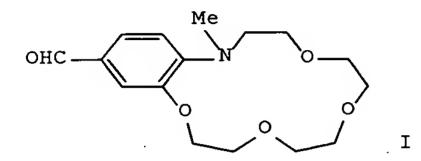
PB Consultants Bureau

DT Journal

LA English

OS CASREACT 131:299435

GI



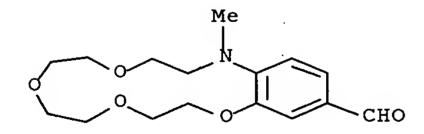
Formyl-substituted benzoazacrown ethers are prepared by ring cleavage of a benzocrown ether with alkylamine to give an aminated podand, which then undergoes derivatization and ring closure to incorporate the aza group into the heterocyclic ring. Thus, 4-formylbenzo-15-crown-5 was cleaved at the ring position para to the formyl group with MeNH2/MeNH3+Cl- to afford a benzene ring-aminated podand with a terminal alc. group on the chain. Treatment of the alc. group of the podand with SOC12/pyridine gave the chloro-substituted derivative which was exchanged with iodide and subsequently cyclized with alkali metal carbonate to give formyl-substituted benzoazacrown ether I. An analog with larger ring size was prepared from 4-formylbenzo-18-crown-6.

IT 247074-86-8P 247074-88-0P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 247074-86-8 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-16-carboxaldehyde, 2,3,5,6,8,9,12,13-octahydro-13-methyl- (9CI) (CA INDEX NAME)



RN 247074-88-0 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-16-carboxaldehyde, 2,3,5,6,8,9,12,13-octahydro- (9CI) (CA INDEX NAME)

RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L5 ANSWER 15 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN
- AN 1998:683632 CAPLUS Full-text
- DN 130:46865
- TI The synthesis of a new cyclodextrin-crown ether chiral stationary phase and application in gas chromatography
- AU Min, Liu; Zhaorui, Zeng; Yuqiang, Ding; Suhuai, Liu
- CS College of Chemistry, Wuhan University, Wuhan, 430072, Peop. Rep. China
- SO Wuhan University Journal of Natural Sciences (1998), 3(3), 337-340 CODEN: WUNSFW; ISSN: 1007-1202
- PB Wuhan University
- DT Journal
- LA English
- AB A new compound of mono-6-(1'-benzo-aza-15-crown-5)-2,3,6-permethyl- β -cyclodextrin (BA-15C5-PM-CD) was synthesized. The structure was studied by IR and NMR spectroscopy. As a stationary phase for capillary gas chromatog., excellent separation for enantiomers and positional isomers was achieved.
- IT 36080-56-5, Benzo-aza-15-crown-5
 - RL: RCT (Reactant); RACT (Reactant or reagent)
 - (in preparation of cyclodextrin-crown ether chiral stationary phase for gas chromatog.)
- RN 36080-56-5 CAPLUS
- CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 2,3,5,6,8,9,12,13-octahydro- (9CI) (CA INDEX NAME)

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 16 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1998:594206 CAPLUS Full-text

DN 130:10049

TI Thermoanalytical studies on crown ether-alkali complexes

AU Pokol, G.; Agai, B.; Tran, T. M. T.; Bitter, I.; Toke, L.; Gal, S.

CS Institute of General and Analytical Chemistry, Technical University of Budapest, Budapest, 1521, Hung.

SO Thermochimica Acta (1998), 319(1-2), 87-95 CODEN: THACAS; ISSN: 0040-6031

PB Elsevier Science B.V.

DT Journal

LA English

AB Solid samples prepared from benzo-15-crown-5, its nitro, acetylamino and decanoylamino derivs. (Group I), and chloro-dibenzo-aza-crown ethers (Group II) with alkali metal salts were studied. The existence of solid adducts between LiBr, NaSCN, KSCN and crown ethers of Group I was proved by DSC. The m.ps. of adducts of the same ligand increase in KSCN<NaSCN<LiBr order. DSC and TG results suggested a ligand scission mechanism of thermal decomposition for all the complexes except that of benzo-15-crown-5 and KSCN where a dissociation and evaporation process took place. The samples prepared from crown ethers belonging to Group II are mech. mixts. of the alkali salts and crown compds.

IT 174628-64-9, 2-Chloro-6,7,9,10,12,13-hexahydro-19H-

dibenzo[b,n][1,4,7,10,13]monoazatetraoxacyclopentadecine

RL: RCT (Reactant); RACT (Reactant or reagent)

(crown ether-alkali complexes detection and ligand:metal molar ratio based thermoanal. studies)

RN 174628-64-9 CAPLUS

CN 19H-Dibenzo[k,n][1,4,7,10,13]tetraoxaazacyclopentadecine, 2-chloro-6,7,9,10,12,13-hexahydro-(9CI) (CA INDEX NAME)

RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 17 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1998:72476 CAPLUS Full-text

DN 128:154071

Vinyl ethers containing an isothiocyanate group. XIII. Ready functionalization of azacrown ethers with 2-(vinyloxy)ethyl isothiocyanate

AU Nedolya, N. A.; Papsheva, N. P.; Trofimov, B. A.

CS Siberian Div., Russian Academy Sciences, Irkutsk Inst. Organic Chemistry, Irkutsk, 664033, Russia

SO Russian Journal of Organic Chemistry (Translation of Zhurnal Organicheskoi Khimii) (1997), 33(2), 143-146 CODEN: RJOCEQ; ISSN: 1070-4280

I

PB MAIK Nauka/Interperiodica Publishing

DT Journal

LA English

GI

 $S = C - NHCH_2CH_2OCH = CH_2$

II

AB Azacrown ethers containing highly efficient vinyloxy and thiocarbamoyl fragments, e.g., I and II, were prepared by the quant. addition of azacrown ethers (aza-12-crown-4, aza-15-crown-5, aza-18-crown-6, benzoaza-15-crown-5, 1,7-diaza-12-crown-4, 1,7-diaza-15-crown-5, 1,10-diaza-18-crown-6, and 1,4-dioxa-7,10,13-triaza-15-crown-5) to 2-(vinyloxy)ethyl isothiocyanate.

IT **36080-56-5**, Benzoaza-15-crown-5

RL: RCT (Reactant); RACT (Reactant or reagent)
(addition reaction with 2-(vinyloxy)ethyl isothiocyanate)

RN 36080-56-5 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 2,3,5,6,8,9,12,13-octahydro- (9CI) (CA INDEX NAME)

RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 18 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1996:294197 CAPLUS Full-text

DN 125:33607

TI Synthesis of dibenzo-monoazacrown ethers

AU Agai, Bela; Nemeth, Valeria; Bocskei, Zsolt; Simon, Kalman; Bitter, Istvan; Toke, Laszlo

CS Department Organic Chemical Technology, Technical University Budapest, Budapest, H-1521, Hung.

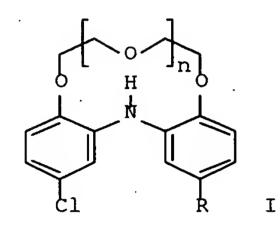
SO Tetrahedron (1996), 52(19), 6713-6724 CODEN: TETRAB; ISSN: 0040-4020

PB Elsevier

DT Journal

LA English

GΙ



Novel dibenzomonoaza-12-crown-3, -15-crown-4, -18-crown-5, and -21-crown-6 derivs. I (n = 1-4, R = H, Cl) were synthesized. Two independent methods were developed for the heterocyclization, and the better one was optimized. The structure of crowns I (n = 1-3, R = H) was confirmed by single-crystal x-ray diffraction.

IT 174628-64-9P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (synthesis of dibenzomonoazacrown ethers)

RN 174628-64-9 CAPLUS

CN 19H-Dibenzo[k,n][1,4,7,10,13]tetraoxaazacyclopentadecine, 2-chloro-6,7,9,10,12,13-hexahydro-(9CI) (CA INDEX NAME)

L5 ANSWER 19 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1996:145679 CAPLUS Full-text

DN 124:216650

TI Interesting conformational and substitutional disorder in the crystal structures of three homologous crowns

AU Bocskei, Zs.; Simon, K.; Nemeth, V.; Agai, B.; Toke, L.

CS Dep. Chem. Res., CHINOIN Res. Cent., Budapest, H-1325, Hung.

SO Acta Crystallographica, Section B: Structural Science (1996), B52(1), 194-200

CODEN: ASBSDK; ISSN: 0108-7681

PB Munksgaard

DT Journal

LA English

The structures of three members of a homologous family of diphenylamine-AB containing crowns, 2-chloro-6,7,9,10-tetrahydro-16Hdibenzo[b,k][1,4,7,10]monoazatrioxacyclododecine (monoclinic, space group P21/a), 2-chloro-6,7,9,10,12,13-hexahydro-19Hdibenzo[b,n][1,4,7,10,13]monoazatetraoxacyclopentadecine (monoclinic, space group P21), 2-chloro-6,7,9,10,12,13,15,16-octahydro-22Hdibenzo[b,q][1,4,7,10,13,16]monoazapentaoxacyclooctadecine (monoclinic, space group Pc), are reported, compared and trends are established. The largest crown (an 18-crown-6-type) presents an ability to form a mol. compound with H2O mols. spontaneously. The propeller-like conformational behavior of the two Ph rings leads to the presence of two chiral conformers in the unit cell of the crystals. Addnl., due to the conformationally nonequiv. role of the two Ph rings, the Cl substitution leads to two further species, resulting in four different conformers in each crystal structure. The presence of so many species in one crystal generates an interesting type of disorder in two of the three cases.

IT 174628-64-9, 2-Chloro-6,7,9,10,12,13-hexahydro-19Hdibenzo[b,n][1,4,7,10,13]monoazatetraoxacyclopentadecine
RL: PRP (Properties)

(crystal structure and conformational anal. of)

RN 174628-64-9 CAPLUS

CN 19H-Dibenzo[k,n][1,4,7,10,13]tetraoxaazacyclopentadecine, 2-chloro-6,7,9,10,12,13-hexahydro-(9CI) (CA INDEX NAME)

L5 ANSWER 20 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1995:942743 CAPLUS Full-text

DN 124:146120

TI Synthesis of heterocyclic crown ethers by intra- versus intermolecular 1,3-dipolar cycloaddition reactions

AU L'abbe, Gerrit; Van Wuytswinkel, Grete; Dehaen, Wim

CS Dep. Chem., Univ. Leuven, Louvain, 3001, Belg.

SO Bulletin des Societes Chimiques Belges (1995), 104(10), 629-30 CODEN: BSCBAG; ISSN: 0037-9646

PB Societe Chimique Belges

DT Journal

LA English

OS CASREACT 124:146120

GI

In the present study we evaluate the use of the 1,3-dipolar cycloaddn. reaction as a tool for the formation of heterocyclic crown ethers. Thus, intramol. cycloaddn. of 2-N3C6H4O(CH2CH2O)3COC.tplbond.CH gave azacrown ethers I and II. Intramol. cycloaddn. of the oxime of 2-OHCC6H4O(CH2CH2O)3CH2C.tplbond.CH gave the isoxazolocrown ether III.

IT 173205-71-5P

RL: BYP (Byproduct); PREP (Preparation)

(preparation of heterocyclic crown ethers via 1,3-dipolar cycloaddns.)

RN 173205-71-5 CAPLUS

CN 4H-[1,2,3]Triazolo[5,1-1][1,4,7,10,13]benzotetraoxaazacyclopentadecin-4-one, 6,7,9,10,12,13-hexahydro-(9CI) (CA INDEX NAME)

L5 ANSWER 21 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1993:81393 CAPLUS Full-text

DN 118:81393

TI Macroheterocycles. IV. Synthesis and analgesic activity of crown ethers containing a Leu-enkephalin and thyroid-releasing hormone fragment

AU Luk'yanenko, N. G.; Basok, S. S.; Kulikov, N. V.; Karaseva, T. L.; Tsapenko, Zh. N.

CS Fiz.-Khim. Inst. im. Bogatskogo, Odessa, Ukraine

SO Khimiko-Farmatsevticheskii Zhurnal (1992), 26(5), 63-6 CODEN: KHFZAN; ISSN: 0023-1134

DT Journal

LA Russian

GI

H-Tyr-D-Ala-Gly-Phe-Leu-N

AB Benzoaza-15-crown-5 and aza-15-crown-5 derivs. containing enkephalin and thyroid-releasing hormone residues, e.g. I, were synthesized. The synthesized compds. administered i.v. had analgesic activity which increased after insertion of a 6-aminohexanoic acid residue between the fragment of enkephalin and benzoaza-15-crown-5. The compound with thyroid-releasing hormone residue had the maximum analgesic effect.

Ι

IT **36080-56-5P**, Benzoaza-15-crown-5

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and peptide coupling reactions of, enkephalin derivs. from)

RN 36080-56-5 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 2,3,5,6,8,9,12,13-octahydro- (9CI) (CA INDEX NAME)

L5 ANSWER 22 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1982:412622 CAPLUS Full-text

DN 97:12622

TI Extraction of metal salts by using macrocyclic crown ethers

AU Gloe, K.; Muehl, P.; Kholkin, A. I.; Meerbote, M.; Beger, J.

CS Zentralinst. Festkoerperphys. Werkstofforsch., DAW, Dresden, 8027, Ger. Dem. Rep.

SO Isotopenpraxis (1982), 18(5), 170-5 CODEN: IPRXA9; ISSN: 0021-1915

DT Journal

LA German

The extraction of alkali, alkaline earth, and transition metal salts by 8 crown ethers was studied at 22°. The extraction order for dibenzo-18-crown-6 is Hg > K > Tl > Ag > Rb > Cs > Na > Sr, but for dicyclohexyl-18-crown-6, it is Hg > Sr > Ag > K > Na. Compns. of extracted complexes include MLn and ML2An while metal complex anions are extracted as M1LM2Am (A = anion, L = crown ether, M = metal).

IT 36080-56-5

RL: PRP (Properties)
 (extraction by, of metal salts)

RN 36080-56-5 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 2,3,5,6,8,9,12,13-octahydro- (9CI) (CA INDEX NAME)

L5 ANSWER 23 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1980:446636 CAPLUS Full-text

DN 93:46636

TI Exchangers with cyclic polyethers as anchor groups. I. Preparation and characterization

AU Blasius, E.; Janzen, K. P.; Keller, M.; Lander, H.; Nguyen-Tien, T.; Scholten, G.

CS Fachrichtung Anorg. Anal. Radiochem., Univ. Saarlandes, Saarbruecken, 6600, Fed. Rep. Ger.

SO Talanta (1980), 27(2), 107-26 CODEN: TLNTA2; ISSN: 0039-9140

DT Journal

LA German

AB Numerous ion exchangers with cyclic polyethers as anchor groups were prepared, and their properties examined 4-(Carboxyethyl)- and 4-(hydroxypropyl)benzo crown ethers were fixed to silica gel and used as stationary phases in high-pressure liquid-chromatog.

IT 74159-04-9P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and properties of)

RN 74159-04-9 CAPLUS

CN Formaldehyde, polymer with 2,3,5,6,8,9,12,13-octahydro-13-methyl-11H-1,4,7,10,13-benzotetraoxaazacyclopentadecine and phenol (9CI) (CA INDEX NAME)

CM 1

CRN 74159-03-8 CMF C15 H23 N O4

CM 2

CRN 108-95-2 CMF C6 H6 O

CM 3

CRN 50-00-0 CMF C H2 O L5 ANSWER 24 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1979:110685 CAPLUS Full-text

DN 90:110685

TI Ligands for the alkali cations. Part 5. Complex formation in solid and solution for some nitrogen crown ligands

AU Blackborow, J. Richard; Lockhart, Joyce C.; Thompson, Maurice E.; Thompson, Derek P.

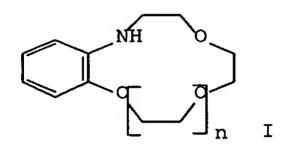
CS Dep. Inorg. Chem., Univ. Newcastle upon Tyne, Newcastle upon Tyne, UK

SO Journal of Chemical Research, Synopses (1978), (2), 53 CODEN: JRPSDC; ISSN: 0308-2342

DT Journal

LA English

GI



The complexing abilities of crown ethers with 1 or 2 O atoms replaced by NH groups were compared by examining the solvent extraction of alkali metal cations with picrate as counterion. Solid NaI complexes were also prepared, but their analyses did not indicate the presence or absence of H2O of crystallization The interaction of N crown ligands is weaker than that of their all-O analogs. Complex formation selectivity varies with ring size, peripheral substituent, and number of NH functions. E.g., I (n = 3, 4) have an improved selectivity for K over Na. The reducing complexing power of the N-containing ligands was attributed to H-bonding of the NH groups with crown ether groups, which may stabilize N crowns, especially in H-bonding solvents.

IT 62871-77-6 62871-78-7

RL: PRP (Properties)

(extraction by, of alkali metals in presence of picric acid)

RN 62871-77-6 CAPLUS

CN 13H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-13-butanoic acid, 2,3,5,6,8,9,11,12-octahydro-γ-oxo- (9CI) (CA INDEX NAME)

RN 62871-78-7 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 2,3,5,6,8,9;12,13-octahydro-13-propyl- (9CI) (CA INDEX NAME)

IT 36080-56-5

RL: PRP (Properties)

(extraction of alkali metals by and crystal structure of)

RN 36080-56-5 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 2,3,5,6,8,9,12,13-octahydro- (9CI) (CA INDEX NAME)

IT 67379-53-7P 67379-54-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 67379-53-7 CAPLUS

CN Sodium(1+), (2,3,5,6,8,9,12,13-octahydro-11H-1,4,7,10,13-benzotetraoxaazacyclopentadecin-N13,O1,O4,O7,O10)-, iodide (9CI) (CA INDEX NAME)

• I.

RN 67379-54-8 CAPLUS

CN Sodium, (2,3,5,6,8,9,11,12-octahydro-γ-oxo-13H-1,4,7,10,13-benzotetraoxaazacyclopentadecine-13-butanoato-N13,O1,O4,O7,O10)-, hydriodide (9CI) (CA INDEX NAME)

L5 ANSWER 25 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1978:571437 CAPLUS Full-text

DN 89:171437

TI Ligands for the alkali metals. Part 4. Nuclear magnetic resonance of crown ethers with alkali-metal ions

AU Lockhart, Joyce C.; Robson, Anita C.; Thompson, Maurice E.; Tyson, Philip D.; Wallace, Ian H. M.

. CS Sch. Chem., Univ. Newcastle upon Tyne, Newcastle upon Tyne, UK

Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1972-1999) (1978), (6), 611-17 CODEN: JCDTBI; ISSN: 0300-9246

DT Journal

LA English

The NMR was studied of benzo-15-crown-5 and benzo-21-crown-7 as free ligands and in mixts. with LiBr, MI (M = Na, K, Rb, CS), or KNCS. The H signals in the mixts. are upfield of those of the free ligand for complexes of 2:1 ligand-cation ratio, but downfield for 1:1 complexes. The shift on complexation is caused by elec. field effect, ring current variations, and specific ion pairing. The conformation of the complexes in solution resembles that found in the crystal.

IT 36080-56-5

RL: PRP (Properties)

(NMR of, in presence of alkali metal salts, complexation in relation to)

RN 36080-56-5 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 2,3,5,6,8,9,12,13-octahydro- (9CI) (CA INDEX NAME)

L5 ANSWER 26 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1977:502392 CAPLUS Full-text

DN 87:102392

TI Macrocyclic hetero imine complexing agents

IN Pedersen, Charles John; Bromels, Marilyn H.

PA du Pont de Nemours, E. I., and Co., USA

SO U.S., 17 pp. Cont. of U.S. 3,847,949.

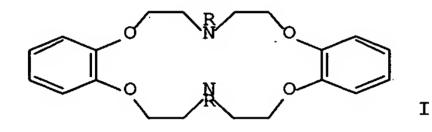
CODEN: USXXAM

DT Patent

LA English

FAN.CNT 3

PATENT NO	. KIND	DATE	APPLICATION NO.	DATE
PI US 403111	1 A	19770621	US 1974-503777	19740906
US 384794		19741112	US 1973-321575	19730108
PRAI US 1970-3	6689 A2	19700512		
US 1973-3	21575 A1	19730108		
GI			•	



Crown, clam, and lantern benzazapolyoxacycloalkenes were prepared for use as metal complexing agents. Thus, o-(HOCH2CH2O)2C6H4 was tosylated, the tosylate treated with PhCH2NH2, o-(PhCH2NHCH2CH2O)2C6H4 condensed with o-(4-MeC6H4SO3CH2CH2O)2C6H4 to give I (R = CH2Ph), which was hydrogenated over Pd-C. The resulting I (R = H) formed a Ag complex with a stability constant 107 L/mol.

IT 36080-57-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and isomerization of)

RN 36080-57-6 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 2,3,5,6,8,9,12,13-octahydro-13-nitroso- (9CI) (CA INDEX NAME)

IT 36080-56-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and nitrosation of)

RN 36080-56-5 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 2,3,5,6,8,9,12,13-octahydro-(9CI) (CA INDEX NAME)

IT 36080-58-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 36080-58-7 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 2,3,5,6,8,9,12,13-octahydro-15-nitroso- (9CI) (CA INDEX NAME)

L5 ANSWER 27 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1977:171416 CAPLUS Full-text

DN 86:171416

TI Ligands for the alkali metals. Part 3. Further examples of

_ nitrogen-containing 'crown' compounds

AU Lockhart, Joyce C.; Thompson, Maurice E.

CS Dep. Inorg. Chem., Univ. Newcastle upon Tyne, Newcastle upon Tyne, UK

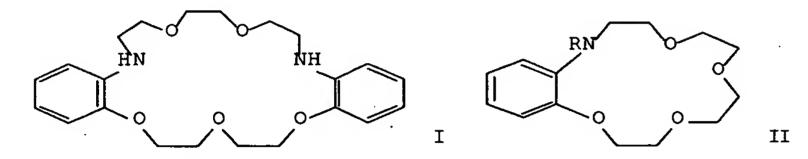
Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1977), (2), 202-4 CODEN: JCPRB4; ISSN: 0300-922X

DT Journal

LA English

OS CASREACT 86:171416

GI



The dibenzocrown I containing 2 secondary amine links was prepared in 4 steps from o-HOC6H4NO2. The monobenzocrown II (R = H) was modified by N-substitution to give II [R = CO(CH2)2CO2H, CO(CH2)2Br]; the bromo compound was reduced to give II [R = Pr, (CH2)3OEt, or (CH2)3Br]. Several other N-containing crown compds. were prepared

IT 62871-75-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reduction of)

RN 62871-75-4 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 13-(3-bromo-1-oxopropyl)-2,3,5,6,8,9,12,13-octahydro-(9CI) (CA INDEX NAME)

IT 62871-77-6P 62871-78-7P 62871-79-8P

62871-80-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 62871-77-6 CAPLUS

CN 13H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine-13-butanoic acid, 2,3,5,6,8,9,11,12-octahydro-γ-oxo- (9CI) (CA INDEX NAME)

RN 62871-78-7 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 2,3,5,6,8,9,12,13-octahydro-13-propyl- (9CI) (CA INDEX NAME)

RN 62871-79-8 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 13-(3-ethoxypropyl)-2,3,5,6,8,9,12,13-octahydro-(9CI) (CA INDEX NAME)

RN 62871-80-1 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 13-(3-bromopropyl)-2,3,5,6,8,9,12,13-octahydro-(9CI) (CA INDEX NAME)

IT 36080-56-5

RL: RCT (Reactant); RACT (Reactant or reagent) (substitution reaction of)

RN 36080-56-5 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 2,3,5,6,8,9,12,13-octahydro- (9CI) (CA INDEX NAME)

L5 ANSWER 28 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1975:525817 CAPLUS Full-text

DN 83:125817

TI Column and thin-layer chromatography of some nitrogen crowns

AU Blackborow, J. R.; Lockhart, J. C.; Minnikin, D. E.; Robson, A. C.; Thompson, M. E.

CS Dep. Inorg. Chem., Univ. Newcastle upon Tyne, Newcastle upon Tyne, UK

SO Journal of Chromatography (1975), 107(2), 380-2 CODEN: JOCRAM; ISSN: 0021-9673

DT Journal

LA English

GI For diagram(s), see printed CA Issue.

AB Synthesized N crown compds. were separated from other components in the oily product obtained by condensation of dichloropolyethers with o-aminophenol or o-phenylenediamine by adsorption on a 30-80 mesh Celite, which was then packed on top of an alumina column and eluted with light petroleum containing increasing amts of Et2O. The eluted fractions were collected, evaporated and monitored by thin-layer chromatog. on Polygram SIL G precoated silica plates by using EtOH or 40:60 Me2CO-light petroleum solvents. The spots were detected in a tank of I vapor. The Rf values of o-aminophenol, 2-morpholinophenol, benzo-12-azacrown-4, and N-(2-hydroxyphenyl)-12- azacrown-4 were 0.79, 0.77, 0.69, and 0.51, resp., when EtOH was used as solvent. When the starting material for the crown compound synthesis was a mixture of dihalides obtained from the action of SOC12 on BDH Polyethylene Glycol 400, compds. I, II, III, and IV were isolated chromatog. from the product and characterized by elemental anal., mass spectrometry, and NMR.

IT 36080-56-5

RL: ANT (Analyte); ANST (Analytical study) (chromatog. of)

RN 36080-56-5 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 2,3,5,6,8,9,12,13-octahydro- (9CI) (CA INDEX NAME)

L5 ANSWER 29 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1975:73049 CAPLUS Full-text

DN 82:73049

TI Macrocyclic hetero imine complexing agents

IN Pedersen, Charles J.; Bromels, Marilyn H.

PA du Pont de Nemours, E. I., And Co.

SO U.S., 14 pp.

CODEN: USXXAM

DT Patent

LA English

FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3847949	Α	19741112	US 1973-321575	19730108
	US 4031111	Α	19770621	US 1974-503777	19740906
PRAI	US 1970-36689	A2	19700512		
	US 1973-321575	A1	19730108		

GI For diagram(s), see printed CA Issue.

The crown compds. I (n = 1,2) and II (X = 0, NH) were prepared by known methods. Lithiation of II (X = 0) and treatment with Br(CH2)10Br gave the clam compound III. Lithiation of II (X = NH) and reaction with o-(p-MeC6H4SO3CH2CH2O)2C6H4 gave the lantern compound IV. II (X = NH) formed as Ag complex with equilibrium constant in H2O of 107 l./mole. IV formed a K complex in MeOH, which had an equilibrium constant of 107±0.3.

IT 36080-57-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and isomerization of)

RN 36080-57-6 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 2,3,5,6,8,9,12,13-octahydro-13-nitroso- (9CI) (CA INDEX NAME)

IT 36080-56-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and nitrosation of)

RN 36080-56-5 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 2,3,5,6,8,9,12,13-octahydro- (9CI) (CA INDEX NAME)

IT 54535-05-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 54535-05-6 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 2,3,5,6,8,9,12,13-octahydro-17-nitroso- (9CI) (CA INDEX NAME)

L5 ANSWER 30 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1973:124560 CAPLUS Full-text

DN 78:124560

TI Preparation of nitrogen-containing polyether crown compounds

AU Lockhart, J. C.; Robson, A. C.; Thompson, M. E.; Sister D. Furtado; Kaura, C. K.; Allan, A. R.

CS Dep. Inorg. Chem., Univ. Newcastle upon Tyne, Newcastle-upon-Tyne, UK

Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1973), (6), 577-81 CODEN: JCPRB4; ISSN: 0300-922X

DT Journal

LA English

GI For diagram(s), see printed CA Issue.

Cl(CH2)20]n(CH2)2Cl (I; n = 1) with o-aminophenols and o-pheny-lenediamines gave the corresponding morpholinophenols and morpholino-amines, resp. E.g. I (n = 1) with 2-H2NC6H4OH (II) gave 2-morpholinophenol. I (n = 2 and 3) with 1,2-(H2N)2C6H4 (III) gave N containing polyether crown compds. E.g. I (n = 3) with III gave 1,2,3,4,5,6,7,8,9,11,13-decahydro-4,7,10,1,13-benzotrioxadiazacyclopentadecin (IV), although I (n = 3) with II also gave 2-(1,4,7-trioxa-10-azacyclododecan-10-yl)-phenol (V). The products were characterized by their spectral properties.

IT 36080-56-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 36080-56-5 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 2,3,5,6,8,9,12,13-octahydro- (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1972:140930 CAPLUS Full-text

DN 76:140930

TI Macrocyclic imines

IN Bromels, Marilyn H.; Pedersen, Charles J.

PA du Pont de Nemours, E. I., and Co.

SO Ger. Offen., 52 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2123256	A	19711223	DE 1971-2123256	19710511
	CA 966127	A1	19750415	CA 1971-109284	19710331
	ES 391018	A1	19740401	ES 1971-391018	19710510
	BE 767022	A1	19711001	BE 1971-103315	19710511
	NL 7106456	Α	19711116	NL 1971-6456	19710511
	FR 2088519	A5	19720107	FR 1971-16967	19710511
	FR 2088519	. B1	19730608		
	BR 7102821	A0	19730417	BR 1971-2821	19710511
	SE 405476	С	19790322	SE 1971-6083	19710511
•	SE 405476	В	19781211		
,	GB 1339667	Α	19731205	GB 1971-14501	19710512
	ES 417898	A 1	19760616	ES 1973-417898	19730814
	SE 7408641	Α	19740701	SE 1974-8641	19740701
	SE 408708	С	19791011		
	SE 408708	, B	19790702		
PRAI	US 1970-36689	Α	19700512		

GI For diagram(s), see printed CA Issue.

The title compds. [e.g., I, X, X1, X2 = NR, O, R = e.g., H, NO, or PhCH2; Q = e.g., (CH2)2, (CH2)3, o-C6H4; or, e.g., II or III] with at least 1 N, several O's separated by 2 or 3 C atoms, and from their configurations named as "crown" (monomacrocyclic, I), "lantern" (bimacrocyclic, II), and "clam" (bridged, III) compds., useful as complexing agents, were prepared Thus, 20.7 g o-H2NC6H4OH and 52.2 g ClCH2(CH2OCH2)4CH2Cl in BuOH was refluxed under N, aqueous NaOH added, and the mixture refluxed to give 9.3 g oily I [X = NH, X1 = X2 = O, Q = (CH2)2]. Eleven other I, II, III, and derivs. thereof were similarly prepared

IT 36080-56-5P 36080-57-6P 36080-58-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 36080-56-5 CAPLUS

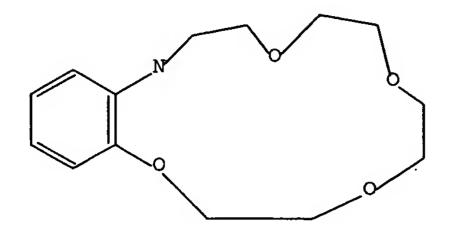
CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 2,3,5,6,8,9,12,13-octahydro- (9CI) (CA INDEX NAME)

RN 36080-57-6 CAPLUS

CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 2,3,5,6,8,9,12,13-octahydro-13-nitroso- (9CI) (CA INDEX NAME)

RN 36080-58-7 CAPLUS
CN 11H-1,4,7,10,13-Benzotetraoxaazacyclopentadecine, 2,3,5,6,8,9,12,13-octahydro-15-nitroso- (9CI) (CA INDEX NAME)

=> d 12; d his; log y L2 HAS NO ANSWERS L1 STR



Structure attributes must be viewed using STN Express query preparation. L2 QUE ABB=ON PLU=ON L1

(FILE 'REGISTRY' ENTERED AT 17:20:28 ON 21 JUL 2005)

DEL HIS Y

L1 STRUCTURE UPLOADED

L2 QUE L1

L3 7 S L2

L4 97 S L2 FUL

FILE 'CAPLUS' ENTERED AT 17:22:33 ON 21 JUL 2005

L5 31 S L4

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
·	ENTRY	SESSION
FULL ESTIMATED COST	154.49	477.79
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-22.63	-22.63

STN INTERNATIONAL LOGOFF AT 17:24:11 ON 21 JUL 2005